Welcome to issue No. 4 of “PURIFAST-News”, semesterly newsletter published within the project in order to keep you informed about its current activities and initiatives, on the main results achieved in industrial and mixed wastewater treatment for water reuse.

In this issue:

Mathematical models and simulation tools to predict and control the efficiency of filtering plants
Outline on the modelling capability to predict filters efficiency

During last two decades many scientists defined models describing the filtration process based on hollow fibres membranes. The model definition is the starting point to develop a numerical code which is able to reproduce the filter behaviour and, therefore, to simulate the evolution in time of its efficiency. Thus, the simulations are an helpful tool to understand and predict the life—time of a filter, avoiding the necessity to set up several experiments.

On the other hand, models and simulations can be considered reliable predicting tools only once they have been validated and tested with experimental data. Therefore, after the model definition, a crucial task is the comparison of the data measured at the plant site: the two activities belonging to this stage (calibration and validation) are often the main difficult and, possibly, they imply a review of the models.

Within the project PURIFAST we used this methodology to provide predicting tools to the industrial partners INGE and POLYMEM. These models are based both on the same assumptions and methods, but each one is specialized for the different filter type. In particular, the definition of the input parameters correspond to the industrial one and so they can be easily set by the user.

In the scientific and technical literature several models to describe the hollow fibres filtration can be found, based on different approaches. One of the main difference lies on the scale at which the problem is addressed, namely microscale or macroscale. The first one studies the problem starting from the description of the fluidynamics occurring inside a single fibres, in order to give a picture of the behaviour and the efficiency of the membrane. For instance, in Fig. 1 we report a typical schematic picture of the process considered at this scale.

Conversely, the macroscopic approach aims to figure out the process taking place in a whole filtering module. Actually, an accurate description requires the definition of a system of partial differential equations accounting for the full 3D problem, even if some simplification due to the geometrical symmetry can be applied. On the other hand, the numerical solution requires a huge time when dealing with long-term simulations corresponding to several days of production.

An alternative method consists in defining a relationship between TMP (trans-membrane pressure) and the membrane resistance, depending only on time. Such a resistance, in turn, is affected by the fouling process. The models belonging to this class are known as resistance in series models: basically they give an averaged description of the process. Because of their reduced complexity, their solution is quick and simple. Nevertheless, very often in these solutions the direct dependency on the module geometry and the membrane structure is lost: in general many unknown parameters are present and an accurate calibration has to be run in order to link this general formulation with the specific device considered.
Within the PURIFAST project we decide to follow an approach representing a sort of “midpoint” between the two methods described above. More in detail, for each filtering device (the hollow fibres and the multi-bore system) we obtained a model depending only on time, but which is the result of an average procedure made on a full 3D model (see, for instance, Fig. 2 for an example of the results obtained with a 3D-modelling approach). Even if the fulfilment of some important assumptions have to be checked in order to guarantee the physical coherence of the model, this approach is a good compromise between the accuracy of a full 3D approach and the standard resistance--in--series methods.

**Fig. 1:** a schematic picture of the typical process taken into account at the micro-scale.

**Fig. 2:** an example of simulation in “quasi-3D” model, at the macro-scale. Here we see the plot of the cake resistance near the inlet at the beginning of the backwash (on the left) and after the backwash (on the right).
Models definition at a glance.

We give here a brief description of the models concepts, without entering in detail. The following considerations are valid for both the INGE and the POLYMEN filtering plants.

- We first define the equations for the evolution of turbidity inside the filter and, consequently, the concentration of matter that has been attached and/or adsorbed in the membrane.
- The attached particles lead to the formation of a cake and so their concentration is linked to the evolution of the so-called cake resistance, which accounts for the reversible fouling.
- The adsorbed particles enter the membrane structure, so that they cause the reduction of porosity and permeability of the membrane. This process cannot be attenuated by the backwash cleaning and it is known as irreversible fouling, represented by a membrane resistance, evolving in time.
- The main equation consists in linking the TMP to the both resistances and such a relationship is the way to evaluate the lowering of the filter efficiency.

The models are defined under the following assumptions and limitations:

1. We assume that only one chemical species soils the membrane, and it represents the whole amount of particles responsible of this phenomenon. Therefore, whenever in the model we consider the “pollutant”, actually we are referring to the turbidity, which is thus the experimental measurement we take into account for what concerns the water quality.
2. We do not represent in the model any chemical cleaning or air scouring process. Anyway, this can be included by resetting the TMP to a lower value at a frequency corresponding to the chemical cleaning stage (or air scouring).
3. No temperature dependence is considered, since we are referring to an experimental device not influenced by thermal effects. Moreover, in general the thermal gradient of the feed water is absolutely negligible.

Calibration

In all the steps cited above, there are some unknown parameters, which can be determined only by calibration: the latter method consists in considering a specific data set and find the best value of these parameters such that the simulation output fits as well as possible the experimental data. Once these values have been found, they can be used to run predicting simulations, even if we have to remind that the general framework cannot be so different to the one considered for calibration. For instance, flux and reference pressure have to be of the same order of magnitude. Consequently, what is really interesting is not the huge variation of the data framework, but the simulation of long—term filtration process, in order to get an estimate of the filter behaviour
avoiding the real production process.

Examples of the models utilization

In Fig. 3 we report two examples of a calibration made on the pilot-plant of POLYMEM and INGE, respectively, at the Baciocavallo site (partner GIDA). We see that we can find a set of parameters such that the simulation can fit both the filtration and the backwash data in a reasonably good way.

The parameters found after the calibration can be fixed and then the process parameters may be changed, within a reasonable range of variance. This step can be an useful tool to get an estimate of the filter behaviour: indeed, even if an experimental assessment is mandatory, this tool is time saving, because it reduces the range of variability of the different process parameters and so the user is somehow directed towards the best configuration.

For instance, in Fig. 4 we report the comparison of the TMP evolution obtained setting two configurations, but taking constant the model parameters, already calibrated. Using data of this type, the user can decide to preserve the energy cost (namely taking the configuration corresponding to the smooth plot) or, conversely, to choose the most efficient configuration in terms of production (namely the steeper graph in the figure).

Another interesting use is the one concerning the estimate of the filter “breakthrough”: in other words, using the selected configuration, the simulation can run out until a threshold of maximum admissible TMP is reached. This method may give to the user a picture of how long the filter can be used without any chemical cleaning or, conversely, to study the best chemical cleaning frequency to avoid the breakthrough.

The following table report an example for the estimate of the time to threshold, computed according to the procedure described above and referred to the pre—industrial plant of INGE at KING COLOR site. The different steps correspond to different data set (basically filtration flow and filtration time are changed).

<table>
<thead>
<tr>
<th>STEP n.</th>
<th>Recovery (%)</th>
<th>Days to threshold</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>78,86</td>
<td>9,7</td>
</tr>
<tr>
<td>2</td>
<td>85,3</td>
<td>5,6</td>
</tr>
<tr>
<td>3</td>
<td>87,4</td>
<td>4,46</td>
</tr>
<tr>
<td>5</td>
<td>89,48</td>
<td>3,65</td>
</tr>
<tr>
<td>6</td>
<td>90,65</td>
<td>2,95</td>
</tr>
<tr>
<td>7</td>
<td>91,58</td>
<td>2,45</td>
</tr>
<tr>
<td>7b</td>
<td>92,32</td>
<td>2,15</td>
</tr>
<tr>
<td>8</td>
<td>93,33</td>
<td>1,31</td>
</tr>
</tbody>
</table>

The evaluation of the best configuration has to be made by finding a good compromise between recovery value and days to threshold.

Moreover, in Fig. 5 we show the TMP plot of configuration n. 2: in this case the filtration can proceed for almost 5 days and half.
Fig. 3. Example of calibration: comparison of the TMP plot obtained by simulation vs the TMP data. Case of POLYMEM (A) and INGE (B) pilot plant at GIDA site of Baciocavallo (Italy).
Fig. 4: simulation of a long-term production using two different configurations. The change in configuration means different flow and filtration times. Case of POLYMEM pilot plant at GIDA site of Baciocavallo (Italy).

Fig. 5: simulation to evaluate the time at which the filter cannot be longer used, unless a chemical cleaning is applied. The threshold value for the TMP is 150 KPa. This example refers to the INGE pilot plant in the KINGCOLOUR site.
Spin-off from the study on modelling hollow fibre filters

The theoretical models and the numerical techniques used in PURIFAST activity have led to interesting generalizations to different application fields, where the hollow fibres are used as well. For instance, in clinical dialysis and in the irrigation of agricultural fields.

As result of this additional activity, we cite the scientific publications describing these studies:

- A. Fasano, A. Farina, Modeling High Flux Hollow Fibers Dialyzers, submitted to *Discrete and Continuous Dynamical Systems - Series B (DCDS-B)*.

For additional info please visit [http://purifast.tecnotex.it/](http://purifast.tecnotex.it/) or send an e-mail to [borsi@math.unifi.it](mailto:borsi@math.unifi.it)